

Nonlinear Model Based Control of Complex Dynamic Chemical Systems

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Abstract

A nonlinear internal model control (NIMC) strategy that incorporates the nonlinear model structure and the estimator dynamics in the control law is presented for the control of complex dynamical systems characterized by input-output multiplicities, nonlinear oscillations and chaos. A model based estimator is designed to provide the unmeasured process states that capture the fast changing nonlinear dynamics of the process to incorporate in the controller. The estimator uses the mathematical model of the process in conjunction with the known process measurements to estimate the states. The design and implementation of the estimator supported NIMC strategy is studied by choosing two typical continuous non-isothermal nonlinear processes, a chemical reactor and a polymerization reactor, which show rich dynamical behaviour ranging from stable situations to chaos. The results evaluated under different conditions show the superior performance of the estimator based NIMC strategy over the conventional controllers for the control of complex nonlinear processes.

Keywords

Nonlinear Control; Oscillatory Dynamics; Chaotic Behaviour; State Estimator; Chemical Reactor; Polymerization Reactor

Introduction

Control of nonlinear systems exhibiting complex dynamic behaviour is a challenging task because such systems present a variety of behavioural patterns depending on the values of their physical parameters and intrinsic features. Among these systems, continuous chemical reactors and continuous polymerization reactors have received special attention due to their complicated dynamics and economic importance. Depending on the parameter values, these systems can be operated at steady state or present oscillatory and chaotic motions. Several researchers have analysed continuous stirred tank chemical reactors to characterize the phenomena of multiple steady states, simple and modulated

oscillations and chaos [Uppal, Ray and Poore, 1976, Schmitzet al., 1979, Doedel and Heinemann, 1983, Blanco and Bandoni, 2007]. Certain continuous polymerization reactors exhibit highly nonlinear dynamics because of the complicated reaction mechanisms associated with the large number of interactive reactions. Many researchers have investigated the existence of steady state multiplicities; self-sustained oscillations and chaos in continuous solution polymerization reactors [Jaisinghani and Ray, 1977, Schmidt et al., 1984, Teymour and Ray, 1989, Flores-Tlacuahuac et al., 2005].

The nonlinear dynamical systems due to variations in the operating parameter space can lead to exhibit open-loop unstable behaviour and some chemical systems are more sensitive to these variations where small perturbation in the operating conditions can cause the stable operation to degenerate into oscillatory and chaotic motion. The unstable, oscillatory and chaotic phenomenon displayed by the chemically reacting systems has desirable as well as undesirable features. The desirable feature of multiple steady state condition is that one of the unstable steady state may correspond to higher rate of reaction/yield and this becomes the preferred state to be operated on it for enhancing the process performance. The desirable feature of chaos is that it enhances mixing and chemical reactions and provides a vibrant mechanism for transport of heat and mass. On the other hand, the intrinsic features of the reacting systems with the interactive influence of chemical or thermal energy may cause irregular dynamic behaviour leading to degraded performance. In such situations, chaotic behaviour is considered as undesirable and should be avoided. Chaotic processes show extreme sensitivity to initial conditions and the process trajectories can diverge exponentially making the task of control more difficult. However, chaos

offers great flexibility to operate chemical systems because there are an infinite number of unstable periodic orbits (UPO) embedded in a chaotic attractor, in which one can choose a specific UPO along with its time averaged pre-specified performance defined in terms of conversion, yield or selectivity and the process can be stabilized to operate it on the chosen UPO. Various conventional and advanced techniques have been reported for the control of open-loop unstable chemical and polymerization reactors and the reactors that show oscillatory and chaotic dynamics. As far as unstable reactors are concerned, Choi and Ray [1988] and Chan et al. [1993] have employed standard PID controllers to stabilize open-loop unstable steady state conditions of an olefin polymerization reactor, however, Takamatsu et al. [1986] and Kwag and Choi [1994] showed that such controllers may also pose serious control problems if the polymerization reactor presents significant nonlinear behaviour. Dittamar et al. [1991] reported that linear predictive controllers might lead to proper control of open-loop unstable polymerization reactor. Various nonlinear model predictive control strategies have been successfully applied to the control of open-loop unstable CSTR systems [Hidalgo and Brosilow, 1990, Hapoğlu, 2002, Venkateswarlu and Venkat Rao, 2005]. Nonlinear processes characterized with chaotic dynamic behaviour can be controlled either by stabilizing the UPOs in the neighbourhood of the desired UPO or stabilizing the dynamic trajectory of the system exactly at the unstable steady state. Various controllers based on ad-hoc, conventional and advanced approaches have been reported to stabilize the chaotic systems. In the ad-hoc approach, the properties of chaos are used to develop ad-hoc methods without considering conventional control techniques. The most commonly used method is the OGY method by which one of the unstable orbits in the chaotic attractor can be stabilized via small time dependent perturbations to a system parameter [Ott et al., 1990, So and Ott, 1995]. The potential difficulty associated with the OGY method is the long transient times before the system enters local region where the perturbation is effective [Petrovet al., 1994]. In conventional control approach, various methods including a proportional-Integral (PI) controller [Pellegrini and Biardi, 1990] and a modified PI/PID controller [Bandyopadhyay, et al., 1997] have been employed for controlling and operating the chaotic reactors under favourable conditions. However, the

complex nature of nonlinear dynamical systems severely limits the use of conventional linear controllers to provide the desired operating performance. In advanced control approach; different nonlinear model predictive controllers have been reported to stabilize the oscillatory and chaotic dynamics in continuous chemical and polymerization reactors [Lima, 1996, Qammaret al., 1996].

Nonlinear control is a class of advanced control in which the nonlinear process model serves as the basis for controller design. This type of control is expected to provide improved control performance since the control structure preserves the nonlinearities of the real process in the form of its mathematical model. The generic model control (GMC) introduced by Lee and Sullivan [1988], the globally linearizing control (GLC) proposed by Kravaris and Chung [1987] and the nonlinear internal model control (NIMC) proposed by Henson and Seborg [1991] are the prominent nonlinear model based controllers. The GMC allows the implementation of the nonlinear process model directly into the controller structure. The GLC is a model based controller that transforms a nonlinear input/output system into a linear input/output system through a nonlinear transformation. The NIMC proposed by Henson and Seborg is different from the GMC of Lee and Sullivan [1988] and the GLC of Kravaris and Chung [1987] in that it includes implicit integral action in the control structure by using the difference between the process output and model output as a feedback signal. A nonlinear filter is employed in NIMC which provides a tuning parameter that can be adjusted for process/model mismatch. Since reasonably accurate mathematical models have been developed to predict the complicated dynamics of nonlinear systems, design of nonlinear controllers based on these models is a useful control alternative for complex dynamical systems. This work is focused towards the model based control of nonlinear dynamical systems in the frame work of NIMC approach. The NIMC approach based controllers have been reported earlier for nonlinear systems where the dynamic behaviour is not so complex [Kurtz and Henson, 1997, Venkateswarlu and Gangiah, 1997].

The objective of this paper is to derive a controller based on NIMC approach for complex dynamical systems that incorporates the nonlinear model structure and the estimator dynamics in the controller formulation. A model based estimator is designed to

provide the unmeasured process states that capture the fast changing nonlinear dynamics of the process to incorporate in the controller. The estimator uses the mathematical model of the process in conjunction with the known process measurements to estimate the states. The design and implementation of the proposed estimator based NIMC strategy is studied by choosing two typical continuous chemical and polymerization reactors that present challenging operational and control problems due to their complex open-loop dynamics such as input-output multiplicities, parametric sensitivity, nonlinear oscillations and chaos. Further the comparison of the estimator based NIMC strategy is made with conventional controllers.

Control Algorithm

The general form of a single input single output (SISO) system with state space description is:

$$\dot{x} = f(x) + g(x)u \quad (1)$$

$$y = h(x) \quad (2)$$

where x is the vector of states, u is the manipulated input, y is the measured output, $f(x)$ and $g(x)$ are vector functions and $h(x)$ is the scalar function. The relative order of the system defined by Eqs. (1) and (2) is expressed by the following relations:

$$L_g L_f^k h(x) = 0, k < r - 1 \quad (3)$$

$$L_g L_f^{r-1} h(x) \neq 0 \quad (4)$$

where r represents the relative order of the system and $L_f h(x)$ is the Lie derivative of the scalar function $h(x)$ with respect to the vector function $f(x)$ with $L_f^0 h(x) = h(x)$. Similarly higher order Lie derivatives as well as the Lie derivative of the scalar function $h(x)$ with respect to the vector function $f(x)$, and then with respect to the vector function $g(x)$ can be defined. The relative order defined by Eqs. (3) and (4) represents the number of times the output y must be differentiated with respect to time so that the input u appears explicitly.

A general form of the control law is written as

$$u = p(x) + q(x)v \quad (5)$$

where v is the new input.

The NIMC approach includes an implicit integral action by using the difference between the plant and model outputs as a feedback signal:

$$e = y_d - (y - \tilde{y}) \quad (6)$$

where $\tilde{y}$ is the process model output. The feedback signal is simplified to $e = y_d$ with perfect model assumption. A nonlinear filter is employed in NIMC which provides a tuning parameter that can be adjusted for process/model mismatch. The new input v for NIMC is defined as

$$v = -\tau_r L_f^{r-1} h(x) - \tau_{r-1} L_f^{r-2} h(x) - \dots - \tau_1 h(x) + \tau_1 e \quad (7)$$

where τ are controller tuning parameters; r is the relative order and $e = y_d$. According to this approach, the control law for the system is given by

$$u = \frac{v - L_f^r h(x)}{L_g L_f^{r-1} h(x)} = p(x) + q(x)v \quad (8)$$

Application Processes

Two typical continuous nonlinear dynamical processes are chosen for the design and implementation of the estimator based NIMC strategy.

Chemical reactor

A non-isothermal, irreversible, first order series reaction $A \rightarrow B \rightarrow C$ in a CSTR with control input and load disturbances is described by the following dimensionless mass and energy balance equations [Kahler et al., 1981]:

$$\frac{dx_1}{dt} = 1 - x_1 - Da x_1 \exp(x_3 / (1 + \varepsilon_A x_3)) + d_1 \quad (9)$$

$$\frac{dx_2}{dt} = -x_2 + Da x_1 \exp(x_3 / (1 + \varepsilon_A x_3)) - Da S x_2 \exp(k x_3 / (1 + \varepsilon_A x_3)) + d_2 \quad (10)$$

$$\frac{dx_3}{dt} = -x_3 + B Da x_1 \exp(x_3 / (1 + \varepsilon_A x_3)) - Da B \alpha S x_2 \exp(k x_3 / (1 + \varepsilon_A x_3)) - \beta(x_3 - x_{3c}) + \beta u_t + d_3 \quad (11)$$

The variables x_1 and x_2 denote the dimensionless concentrations of species A and B respectively, and x_3 is the dimensionless temperature. The parameter x_{3c} represents the reactor coolant temperature. An externally manipulated variable u_t can be defined to denote a measure of the deviation in the coolant temperature from the reference value x_{3c} . The load disturbances in feed compositions are denoted by d_1 and d_2 , and the load disturbance in the reactor

temperature is denoted by d_3 . This reactor system exhibit multi-stationary behaviour, oscillations and chaos for the parameter values shown in Table 1.

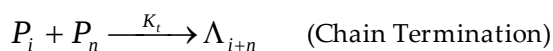
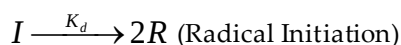
TABLE 1 CHARACTERIZATION OF STEADY STATES

Set No	Parameter values	x_{1s}	x_{2s}	x_{3s}	Stability
I	$Da=0.06, S=0.0005, \varepsilon A=0, k=1, \alpha=0.426, \beta=7.7, B=55.0$	0.0378	0.9501	6.0500	Unstable
II	$Da=0.26, S=0.5, \varepsilon A=0, k=1, \alpha=0.426, \beta=7.7, B=57.77$	0.0729	0.1259	3.8902	Stable limit cycle
III	Same as Set II except $\beta=7.9999$	0.0819	0.1391	3.7627	Chaotic

Homopolymerization reactor

Continuous homopolymerization reactors represent one important class of dynamical systems. The homopolymerization reactions are characterized by high heat release, high viscosity and poor heat transfer. Vinyl acetate homopolymerization has shown complex dynamic behaviour for certain ranges of operating conditions due to the large heat of polymerization, the gel effect and the large activation energy of the initiation step. These factors can readily produce phenomena such as multiple steady states, steady state instability, limit cycles and chaos.

The kinetic mechanism for free-radical vinyl acetate homopolymerization reaction is as follows.



The mathematical model for homopolymerization reaction of vinyl acetate in tertiary butanol using AIBN as initiator is described by the following equations [Pinto and Ray, 1995]:

Monomer Mass Balance

$$\frac{dv_m}{d\tau} = \frac{\rho_{mf} v_{mf}}{\rho_m} - q_o q_i v_m - \frac{(MW)_m R_m \theta}{\rho_m} + v_m \rho_m \frac{dT}{d\tau} \frac{d(1/\rho_m)}{dT} \quad (13)$$

Solvent Mass Balance

$$\frac{dv_s}{d\tau} = \frac{\rho_{sf} v_{sf}}{\rho_s} - v_s q_o q_i + \rho_s v_s \frac{dT}{d\tau} \frac{d(1/\rho_s)}{dT} \quad (14)$$

Initiator Mass Balance

$$\frac{dc_i}{d\tau} = c_{if} - c_i (q_o q_i + k_d \theta) \quad (15)$$

Energy Balance

$$\frac{dT}{d\tau} = \frac{\rho_f (T_f - T)}{\rho} + \frac{\theta}{\rho C_p} \frac{\Delta H}{(MW)_m} v_m \rho_m k_p P - \frac{\theta}{\rho C_p} \frac{UA(T - T_c)}{V} + \beta u_t \quad (16)$$

In the above equations, $q_o q_i$ is a term that takes into account changes in the density of the reactive mixture and is defined by

$$q_o q_i = \frac{\rho_{mf} v_{mf}}{\rho_m} + \frac{\rho_{sf} v_{sf}}{\rho_s} + \theta (MW)_m \rho_m R_m \left(\frac{\rho_m}{\rho_p} - 1 \right) + \frac{dT}{d\tau} \left(\rho_s v_s \frac{d(1/\rho_s)}{dT} + \rho_m v_m \frac{d(1/\rho_m)}{dT} + \rho_p v_p \frac{d(1/\rho_p)}{dT} \right) \quad (17)$$

$$\text{and } \beta = \frac{\theta}{\rho C_p} \frac{UA}{V}.$$

The overall density and specific heat of the mixture are

$$\rho = \rho_m v_m + \rho_s v_s + \rho_p v_p$$

$$C_p = y_m C_{pm} + y_s C_{ps} + y_p C_{pp}$$

Under quasi steady state assumption for the free-radical species (R and P), the normalized rate of monomer reaction is expressed as

$$Rate_m = k_p P + R_{ckr} \quad (18)$$

where concentration of species P can be written as

$$P = \sqrt{\frac{R_{ckr} M}{k_t}} \quad (19)$$

The R_{ckr} is the normalized rate of initiation as given by

$$R_{ckr} = \frac{2fk_d c_i}{M} \quad (20)$$

By substituting the value of R_{ckr} from Eq. (20) in Eq. (18), we have

$$\begin{aligned} \text{Rate}_m &= k_p P + \frac{2fk_d c_i}{M} \\ &= \frac{R_m (MW)_m}{\rho_m v_m} \end{aligned} \quad (21)$$

where R_m is the rate of monomer consumption expressed by

$$R_m = \frac{k_p P \rho_m v_m}{(MW)_m} + 2fk_d c_i \quad (22)$$

The termination and propagation constants (k_t, k_p) used in the above equations include gel effect with the form

$$\begin{aligned} k_t &= k_t^0 g_t \\ k_p &= k_p^0 g_p \end{aligned} \quad (23)$$

The gel effect correlations are

$$\begin{aligned} g_p &= 1 \\ g_t &= \exp(-0.4407x_t - 6.753x_t^2 - 0.3495x_t^3) \end{aligned}$$

In Eq. (23), k_t^0 and k_p^0 are the kinetic constants at zero polymer concentration, g_t and g_p are the gel effect

TABLE 2 VA HOMOPOLYMERIZATION SYSTEM PARAMETERS

$f = 0.8$
$V = 500$ (ml)
$UA = 12$ (cal/min K)
$\Delta H = 21000$ (cal/gmol)
$C_{pm} = 0.470$ (cal/g K)
$C_{ps} = 0.716$ (cal/g K)
$\rho_m(T) = 958.4 - 1.3276(T - 273)$ (g/lit)
$\rho_p(T) = 1211 - 0.8496(T - 273)$ (g/lit)
$\rho_s(T) = \left(\frac{74120}{(60.21 + 0.116T)} \right)$ (g/lit)
$C_{pp} = 0.3453 + 9.55 \times 10^{-4}(T - 298)$ (cal/g K)
$k_p^0 = 82.212 \times 10^8 e^{\frac{-6100}{RT}}$ (lt/gmol.s)
$k_d = 94.8 \times 10^{15} e^{\frac{-30800}{RT}}$ (lt/gmol.s)
$k_t^0 = 469.392 \times 10^{10} e^{\frac{-2462}{RT}}$ (lt/gmol.s)

correlations that take into account the effects of increasing polymer concentration. The other parameters necessary for simulation are presented in Table 2.

Design of Estimator Based Nonlinear Controller

The nonlinear internal model controller (NIMC) relies on mathematical model of the process incorporating process state variable information in the controller formulation. Since the state variables desired by the controller are not easily available through measurement or available with large measurement delays, a model based nonlinear estimator is designed to provide the unmeasured states needed by the controller.

Controller Design

The design of NIMC for complex dynamic processes considered in this work is briefed as follows:

1) Chemical Reactor

The $f(x)$ and $g(x)$ in Eq. (1) can be written by omitting the load disturbances from the dimensionless mass and energy balances in Eqs. (9) - (11):

$$f(x) = \begin{bmatrix} 1 - x_1 - Da x_1 \exp\left(\frac{x_3}{1 + \varepsilon_A x_3}\right) \\ -x_2 + Da x_1 \exp\left(\frac{x_3}{1 + \varepsilon_A x_3}\right) - Da S x_2 \exp\left(\frac{k x_3}{1 + \varepsilon_A x_3}\right) \\ -x_3 + BDa x_1 \exp\left(\frac{x_3}{1 + \varepsilon_A x_3}\right) - BDa a S x_2 \exp\left(\frac{k x_3}{1 + \varepsilon_A x_3}\right) - \beta x_3 \end{bmatrix} \quad (24)$$

$$g(x) = \begin{bmatrix} 0 \\ 0 \\ \beta \end{bmatrix} \quad (25)$$

The controlled output in Eq. (2) is given by

$$y = h(x) = x_3 \quad (26)$$

From Eqs. (3) and (4), the relative order of the system is evaluated as one. Thus for $r=1$, the new input v in Eq. (7) is obtained as

$$v = \tau_1(x_3^s - x_3) \quad (27)$$

On computing the Lie derivatives and substituting them along with the new input in Eq. (8) leads to the following control law

$$u_t = \frac{\tau_1(x_3^s - x_3) - \left(-x_3 + BD\alpha x_1 \exp\left(\frac{x_3}{1 + \varepsilon_A x_3}\right) - BD\alpha\alpha Sx_2 \exp\left(\frac{kx_3}{1 + \varepsilon_A x_3}\right) - \beta x_3 \right)}{\beta} \quad (28)$$

where α is the NIMC tuning parameter.

The $f(x)$ and $g(x)$ in Eq. (1) can be defined from the mass and energy balances of Eqs. (13) - (16):

2) Polymerization reactor

$$f(x) = \begin{bmatrix} \frac{\rho_m v_m}{\rho_m \theta} - \frac{q_o q_i v_m}{\theta} - \frac{(MW)_m R_m}{\rho_m} + v_m \rho_m \frac{d(1/\rho_m)}{dT} \left(\frac{\rho_f (T_f - T)}{\rho} + \frac{\theta}{\rho C_p (MW)_m} v_m \rho_m k_p P - \frac{\theta}{\rho C_p} \frac{UA(T - T_c)}{V} \right) \\ \frac{\rho_s v_s}{\rho_s \theta} - \frac{q_o q_i v_s}{\theta} + \rho_s v_s \frac{d(1/\rho_s)}{dT} \left(\frac{\rho_f (T_f - T)}{\rho} + \frac{\theta}{\rho C_p (MW)_m} v_m \rho_m k_p P - \frac{\theta}{\rho C_p} \frac{UA(T - T_c)}{V} \right) \\ \frac{c_{if}}{\theta} - \frac{q_o q_i}{\theta} c_i - k_d c_i \\ \frac{\rho_f (T_f - T)}{\theta \rho} + \frac{\Delta H v_m \rho_m k_p P}{\rho C_p (MW)_m} - \frac{UA(T - T_c)}{V \rho C_p} \end{bmatrix} \quad (29)$$

$$g(x) = \begin{bmatrix} 0 \\ 0 \\ 0 \\ \beta \end{bmatrix} \quad (30)$$

The controlled output in Eq. (2) is obtained as

$$y = h(x) = T \quad (31)$$

The conditions in Eqs. (3) and (4) defining the

polymer reactor system is of relative order one. The new input v in Eq. (7) is computed as

$$v = \tau_1(T_s - T) \quad (32)$$

$$u_t = \frac{\tau_1(T_s - T) - \left(\frac{\rho_f (T_f - T)}{\theta \rho} + \frac{\Delta H v_m k_p \rho_m P}{\rho C_p (MW)_m} - \frac{UA(T - T_c)}{V \rho C_p} \right)}{\beta} \quad (33)$$

Estimator Design

The success of estimator based controller for nonlinear dynamical systems relies on the performance of the estimator as well as the model of the process that supports the estimator. Since mathematical models with enough details are used to develop the NIMC strategy for complex dynamical systems, it is advantageous to use the same models in the estimator design in order to obtain fast and accurate estimation of unmeasured process states desired by the controller. Recently, model based estimators have been successfully employed for state estimation in various stable systems [Venkateswarlu and Gangiah, 1992, Schuler and Schmidt, 1993, Sargantanis and Karim,

1994, Aguilar-López and Martinez-Guerra, 2005]. In this work, a nonlinear model based estimator known as extended Kalman filter (EKF) is designed to obtain the state estimates from the known temperature measurements of the respective processes. The estimator design for NIMC strategy of this work is similar to that of the recently reported estimator involved in the GLC control of a chaotic chemical reactor [Karri et al., 2009, Karri, 2011]. The general process representation for model based state estimation is given in Appendix A. The EKF estimation algorithm is given in Appendix B. The elements of the state transition and measurement matrices involved in the estimator are given in

Appendix C.

Results and Discussion

Chemical Reactor

The reactor system described by Eqs. (9)-(11) exhibits multi-stationary behaviour, oscillations and chaos for parameter values given as sets I, II and III, respectively, in Table. 1. For parameter set I, the system shows unstable steady state, where as for parameter sets II and III, the system exhibits limit cycle oscillations and chaotic behaviour. The temperature data used for state estimation are obtained through numerical integration of model equations using Gear's method with a sampling time of 0.0001 units. A model based state estimator, extended Kalman filter is employed to estimate the states x_1 , x_2 and x_3 using the temperature measurement of the reactor. The performance of the EKF estimator is evaluated by considering different cases of process parameter values shown in Table 1. The results in Fig. 1 represent the phase plane plots of the actual and estimated states of CSTR corresponding to the parameter values in set III.

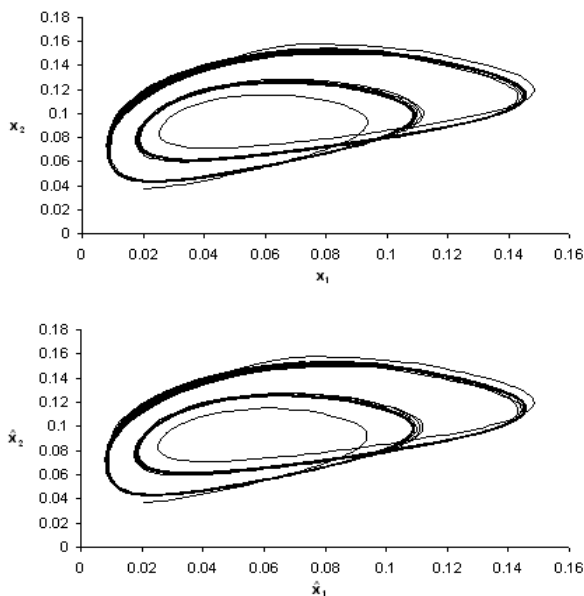


FIG. 1. ACTUAL (x_1, x_2) AND ESTIMATED $(\hat{x}_1, \hat{x}_2)$ PHASE PLANE PLOTS FOR SET – III

Fig. 2 shows the actual and estimated concentration profiles corresponding to set III in the presence of stochastic noise in temperature obeying Gaussian distribution. Similar results are evaluated for set I and set II. In all the cases, the estimated states are in close resemblance with the actual states.

The NIMC strategy supported by the state estimator is

applied with the objectives of controlling the chemical reactor at an unstable steady state in the multiplicity region, at the unique unstable steady state responsible for limit cycle oscillations and at unique unstable steady state responsible for chaotic motion. The controller parameter involved in NIMC is tuned as $\pi=14.0$ based on objective function to minimize the integral of absolute error (IAE). The results are also compared with those of a modified PID controller with feedback mechanism, which has the form given by [22],

$$\frac{du_t}{dt} = \varepsilon_0 f'(t)e + \varepsilon_0 f(t) \frac{de}{dt} + \varepsilon_1 \int e dt \quad (34)$$

where $f(t)=t$ and $f'(t)=1$. The tuning parameters of the PID controller (a, a) are evaluated using Ziegler-Nichols method. A sampling time of 1 sec is used for the implementation of the estimator and the controller. For parameter values in set I, the system exhibits multiple steady state behaviour. The controller goal is to shift the process operating at an arbitrary point ($x_{10} = 0.04$, $x_{20} = 0.9$, $x_{30} = 5.75$) to the set condition in Table 1 and maintain it at that state.

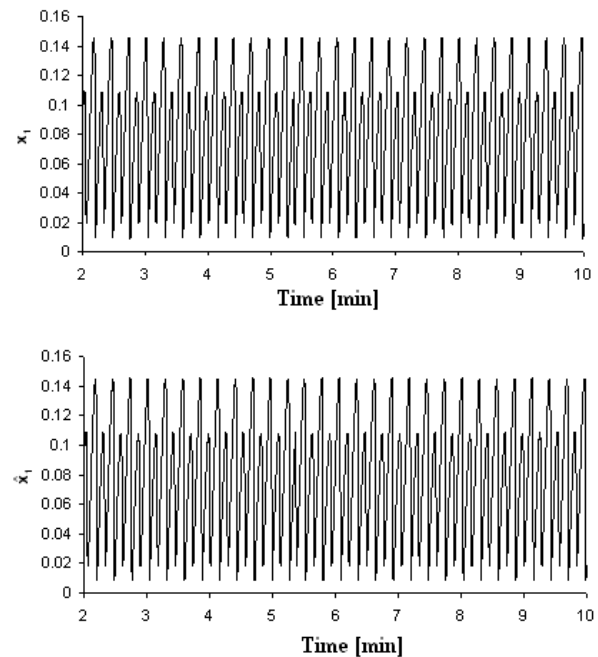


FIG. 2. ACTUAL (x_1) AND ESTIMATED $(\hat{x}_1)$ CONCENTRATION PROFILES FOR SET-III IN THE PRESENCE OF STOCHASTIC DISTURBANCE

Fig. 3 shows the process output and controller output plots of NIMC and PID controller, respectively for this condition. For parameters in set II, the system exhibits sustained oscillatory behaviour (stable limit cycle) and the controllers are also required to regulate the

trajectory at the unique unstable steady state, which is the desired condition. Fig. 4 shows the results of the NIMC and PID controller to realize the set condition in Table 1 from an arbitrarily selected initial state ($x_{10} = 0.08$, $x_{20} = 0.103$, $x_{30} = 3.654$). For parameters in set III, the system exhibits chaotic behaviour. In this objective, the controller has to stabilize the chaotic trajectory exactly at the corresponding unique unstable steady state. To realize this objective, the controllers are also applied using the same initial condition as in set II to satisfy the desired condition for set III given in Table 1.

The process output and controller output plots of NIMC and modified PID controller corresponding to this objective are shown in Fig. 5. These plots indicate that the controllers fulfil the desired objectives without any offset. The nonlinear controller has shown better stabilization over PID controller. The performance of the controllers is also evaluated by applying them for controlling the system at the desired conditions in the presence of deterministic and stochastic load

disturbances. A deterministic disturbance of 1.0 and a stochastic load disturbance generated through random Gaussian noise of zero mean and a standard deviation of 0.25 are considered to represent the d_3 in temperature measurement. The results of the controllers for stabilizing the system at unstable steady state responsible for chaotic motion with these disturbances conditions are shown in Figs. 6 and 7.

These results indicate the better performance of the NIMC strategy in the presence of either type of load disturbances. The results of the controllers are also evaluated for a series of step changes in the set points of the controlled variables. The results in Fig. 8 show the process output and controller output plots of NIMC and modified PID controller for parameters in set III for a series of $\pm 20\%$ step changes in the set conditions in Table 1. These results show the better performance of the estimated supported nonlinear controller.

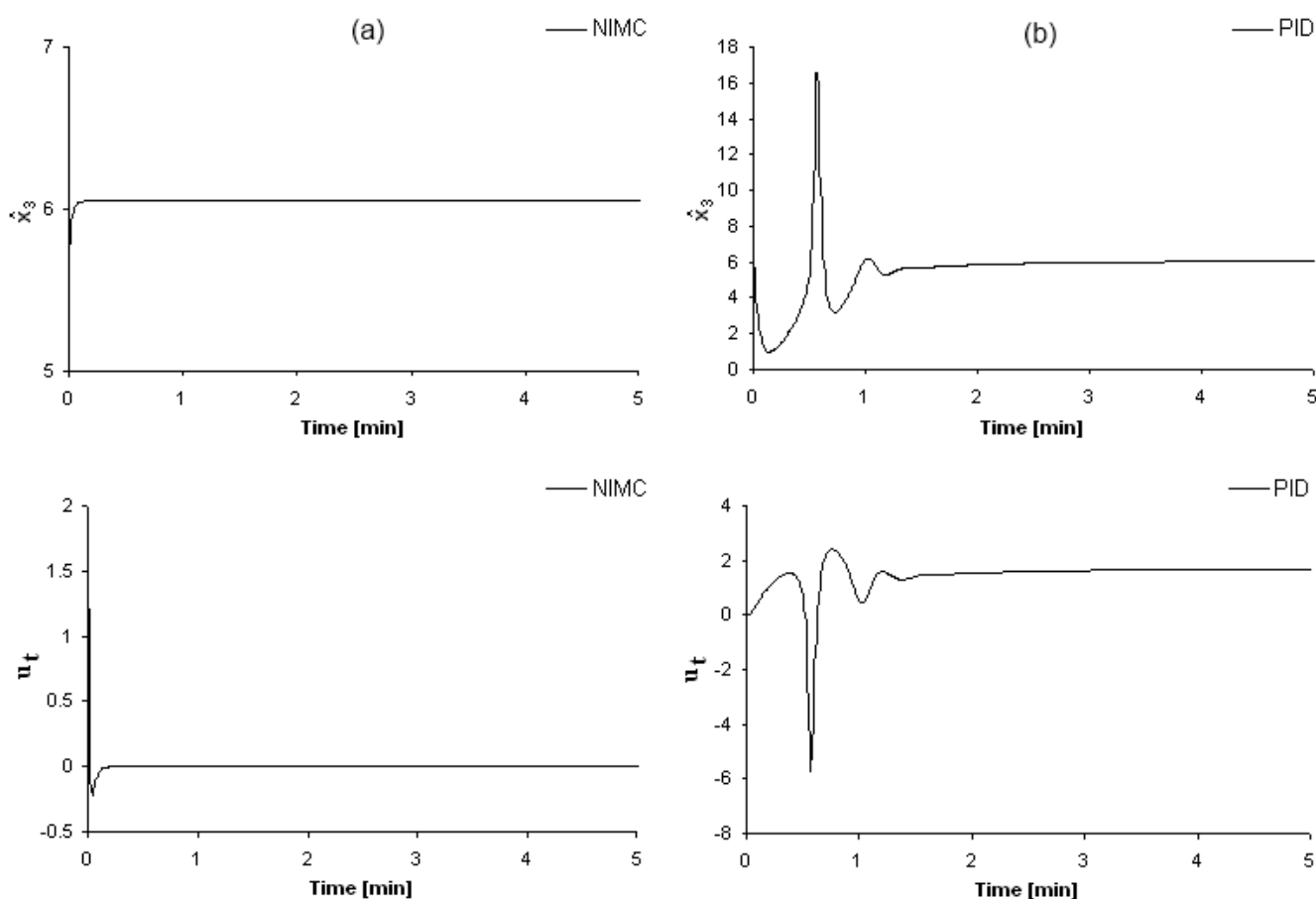


FIG. 3 PROCESS AND CONTROLLER OUTPUT PLOTS FOR SET I OF (A) NIMC AND (B) PID

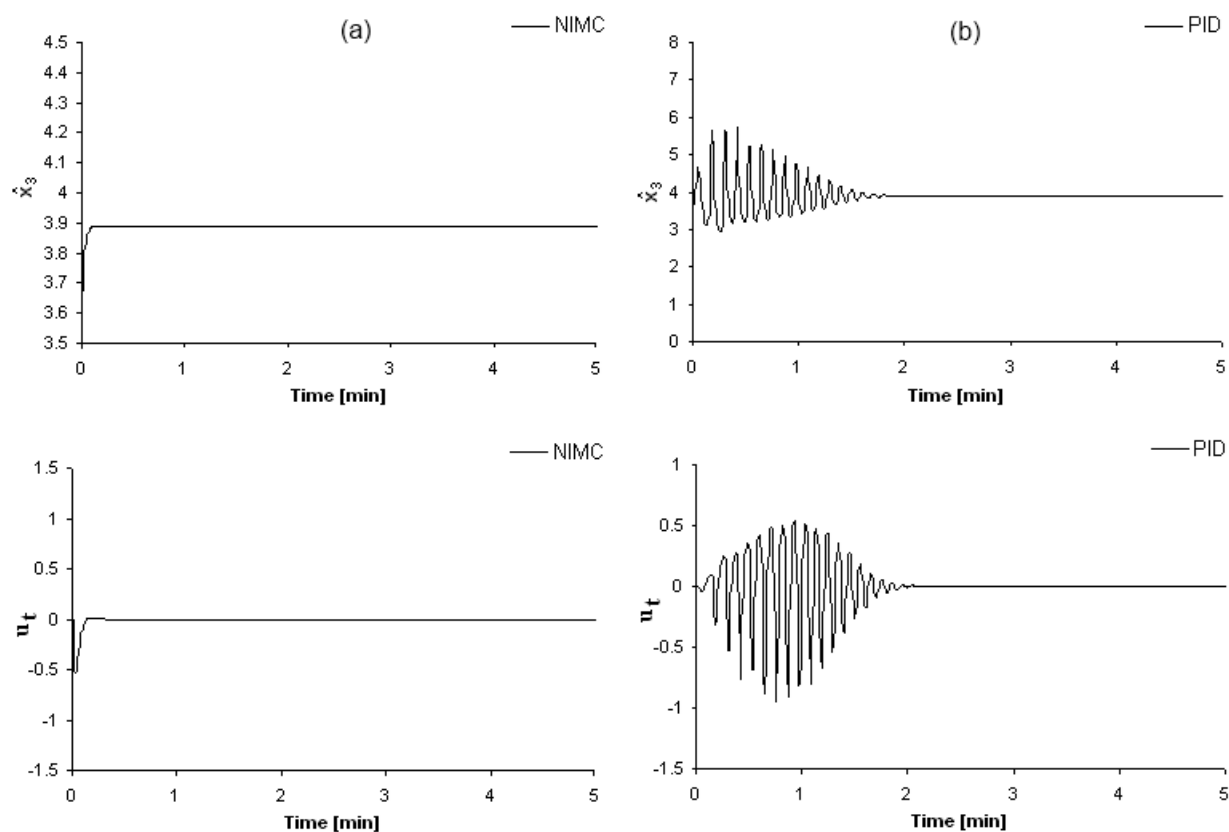


FIG. 4 PROCESS AND CONTROLLER OUTPUT PLOTS FOR SET II OF (A) NIMC AND (B) PID

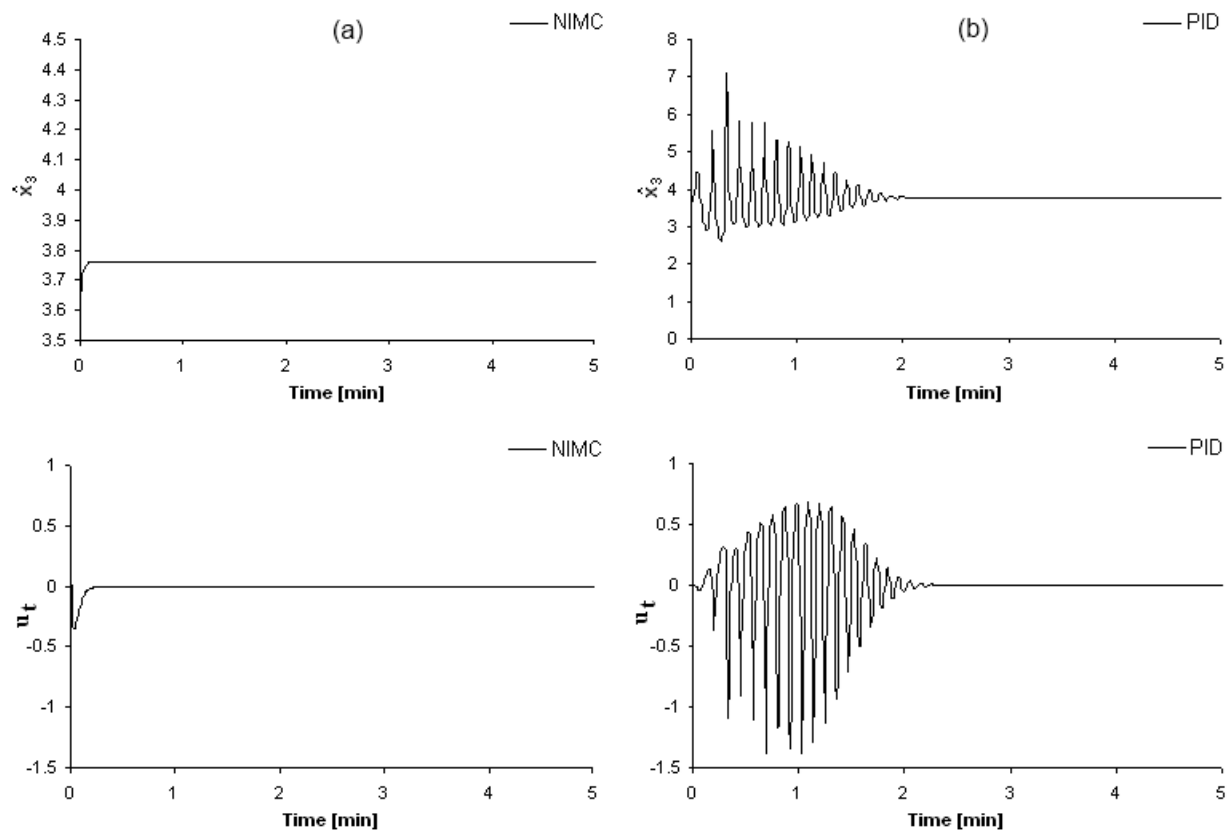


FIG. 5 PROCESS AND CONTROLLER OUTPUT PLOTS FOR SET III OF (A) NIMC AND (B) PID

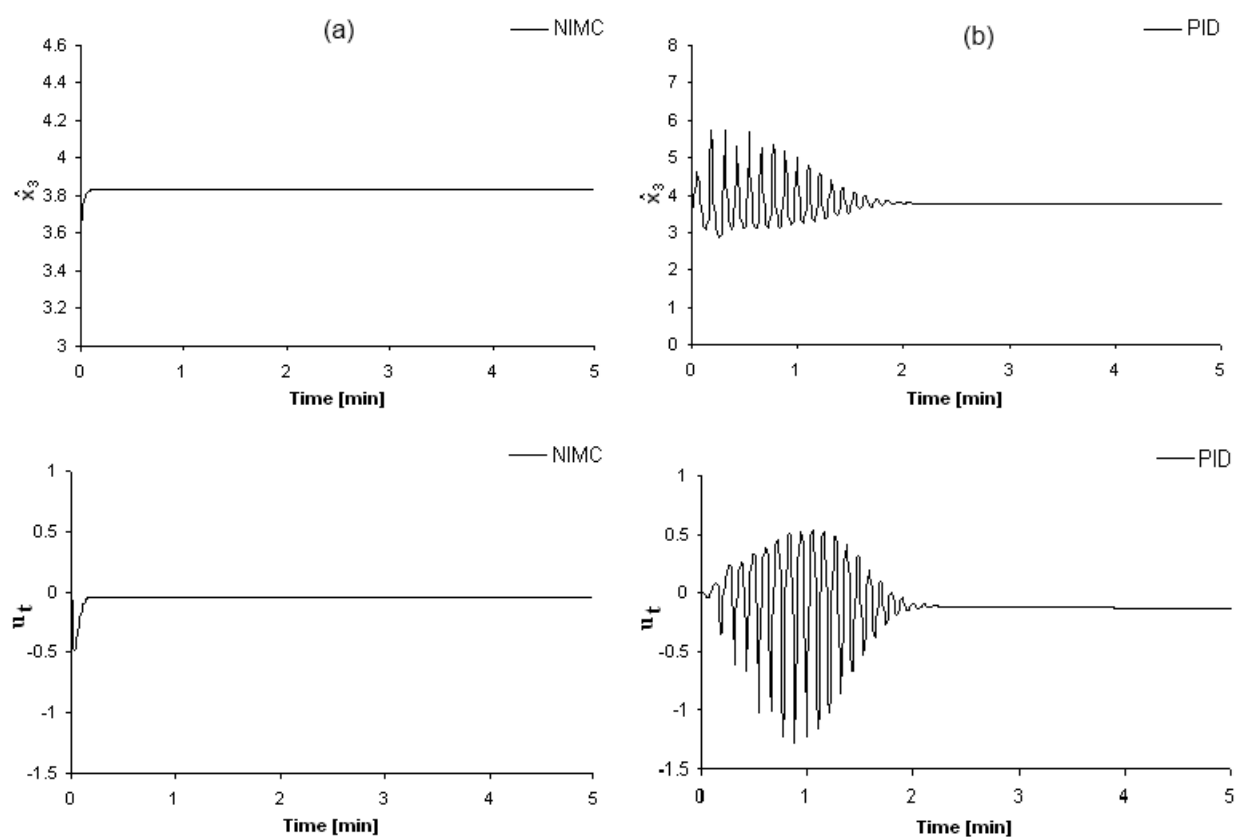


FIG. 6 PROCESS AND CONTROLLER OUTPUT PLOTS OF NIMC AND PID WITH DETERMINISTIC DISTURBANCE FOR SET III

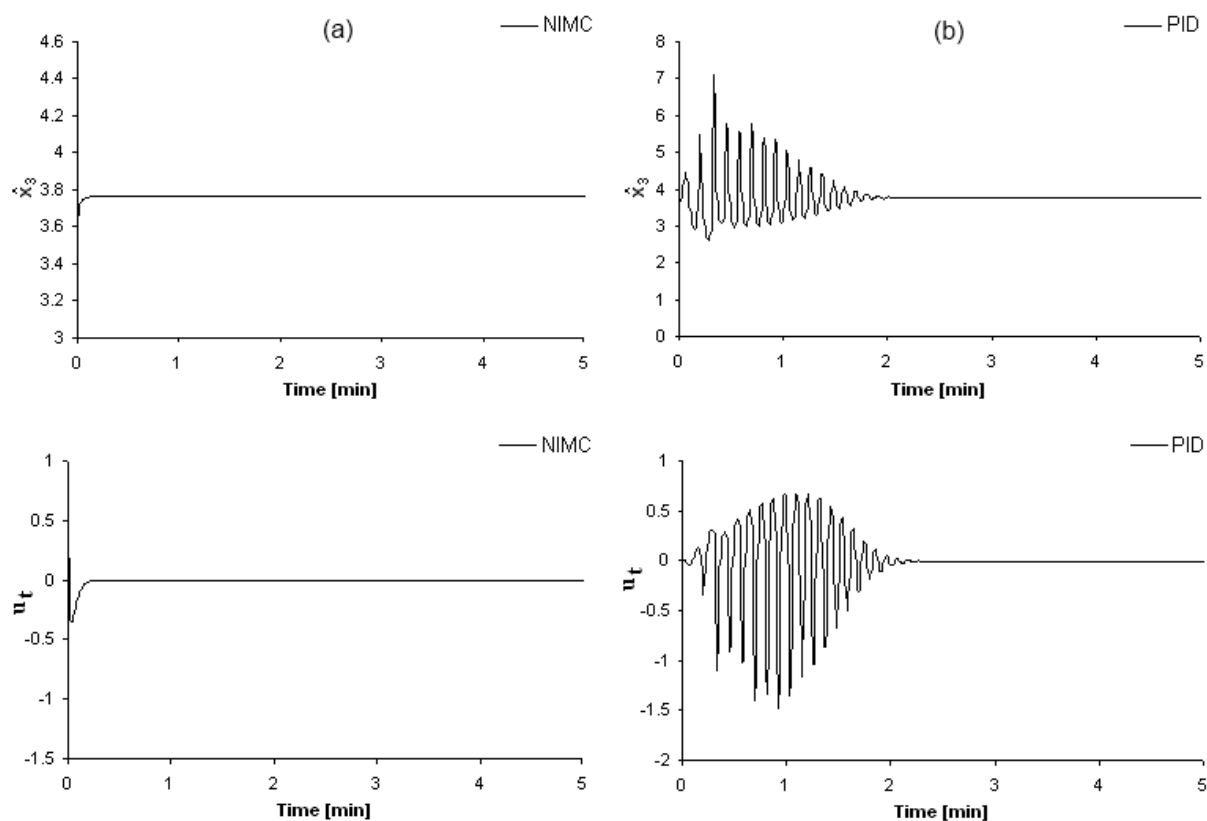


FIG. 7 PROCESS AND CONTROLLER OUTPUT PLOTS OF NIMC AND PID WITH STOCHASTIC DISTURBANCE FOR SET III

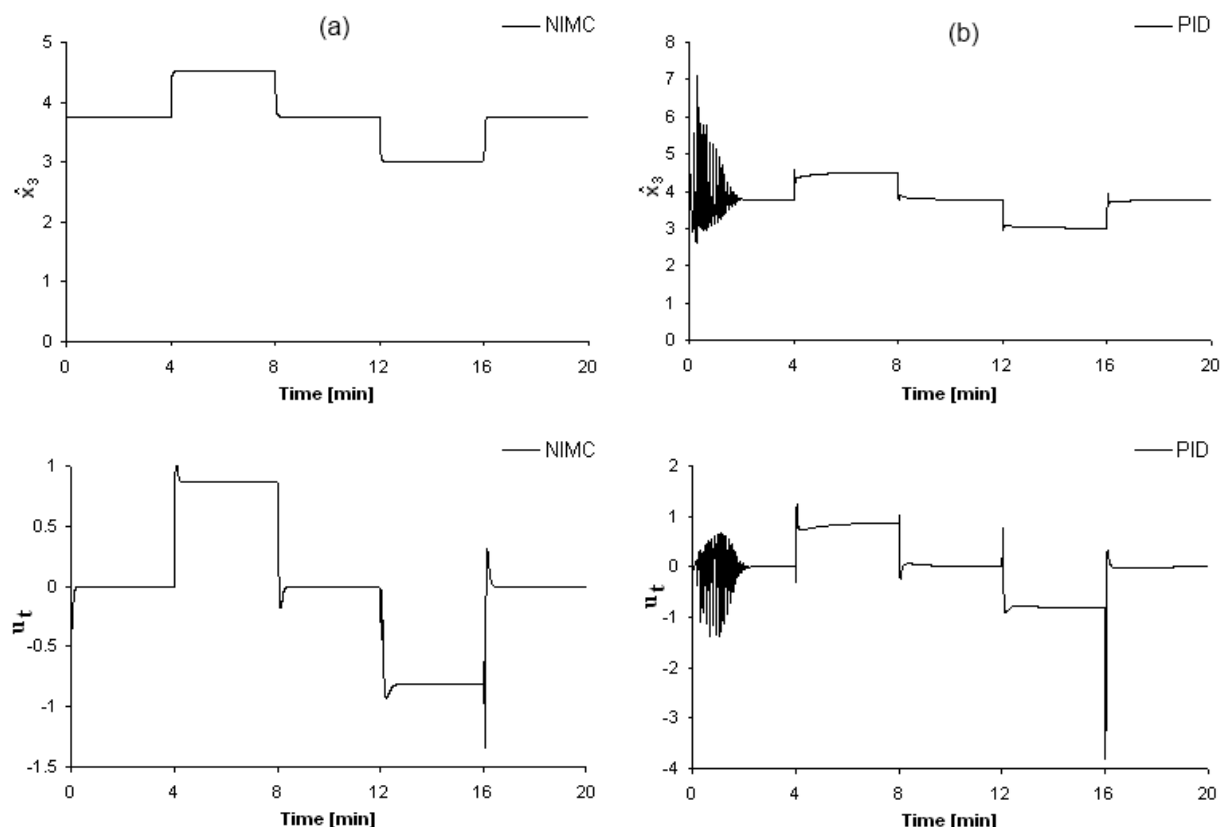


FIG. 8 PROCESS AND CONTROLLER OUTPUT PLOTS OF NIMC AND PID FOR A SERIES OF STEP CHANGES IN SET POINTS OF THE CONTROLLED VARIABLES FOR SET III

Polymerization Reactor

The mathematical model of homopolymerization reactor is solved by numerical integration using Gear's method with a sampling time of 0.0001 units. The bifurcation diagram of VA homopolymerization shown in Fig. 9 drawn for the operating conditions, $T_c = 318$ K, $T_f = 315$ K, $v_{mf} = 0.3$ and $c_{if} = 0.03203$ gmol/l, presents the existence of multiple steady states, limit cycle and bifurcation points as well as stable and unstable zones with respect to the variation of residence time.

From Fig. 9, it can be observed that the transition occurs from stable to unstable zone beginning at $\theta = 24$ min. This transition causes oscillatory behaviour in response that eventually lead to period doubling bifurcation cascade and chaos as shown in Fig. 10(a). The magnification results of Fig. 10(a) are further explained in Figs. 10(b) and 10(c), which show the sequence of periodic windows of periods 2, 4, 8 and so on leading to chaotic region. At $\theta = 27.37$ min, the chaotic behaviour with huge temperature oscillations is observed as shown in Fig. 11. The time domain response is shown in Fig. 11(a) and the corresponding

phase plane plot is depicted in Fig. 11(b).

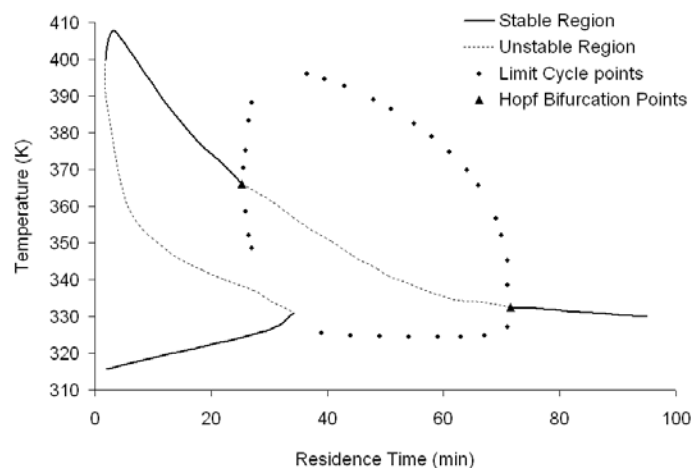


FIG. 9 PERIOD DOUBLING BIFURCATION DIAGRAM

A model based estimator, extended Kalman filter (EKF) is employed to estimate the states v_m vs c_i and T using the temperature measurement of the reactor. The performance of the estimator is evaluated under different conditions. Fig. 12 compares the actual and estimated results of VA homopolymerization reactor. These results confirm the usefulness of the method of EKF as a state estimator for polymerization reactor.

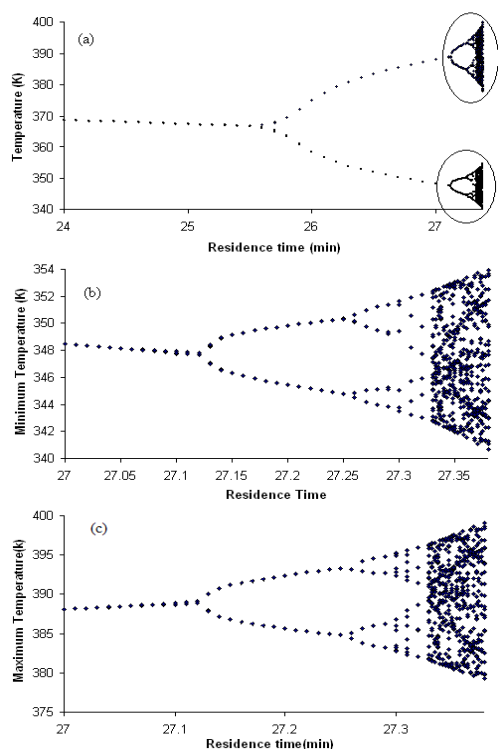


FIG. 10 ONE DIMENSIONAL POINCARÉ BIFURCATION DIAGRAM: (A) TRANSITION FROM LIMIT CYCLES TO CHAOS, (B) MINIMUM TEMPERATURE AND (C) MAXIMUM TEMPERATURE

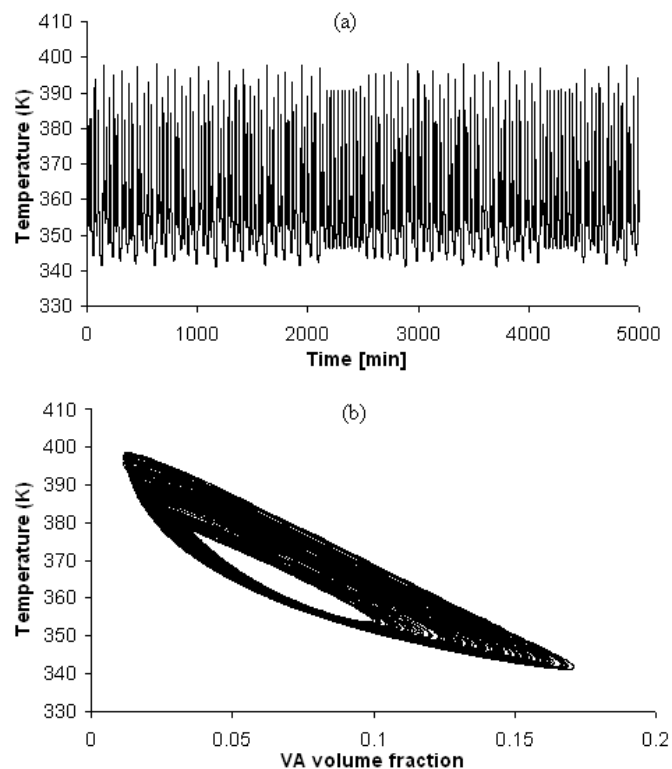


FIG. 11 CHAOTIC BEHAVIOUR (A) TIME DOMAIN RESPONSE, (B) PHASE PLANE PLOT

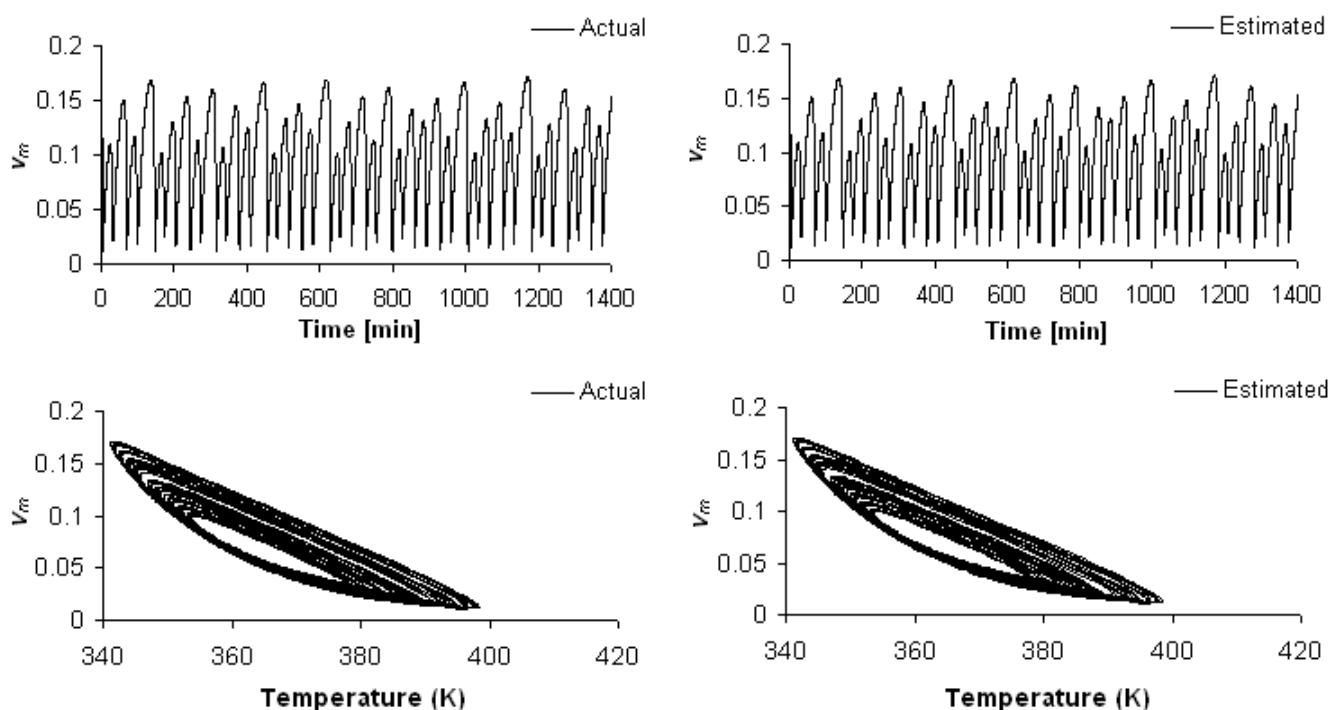


FIG. 12 ACTUAL AND ESTIMATED PROFILES OF MONOMER VOLUME FRACTION (A) TIME DOMAIN RESPONSE (B) PHASE PLANE PLOTS

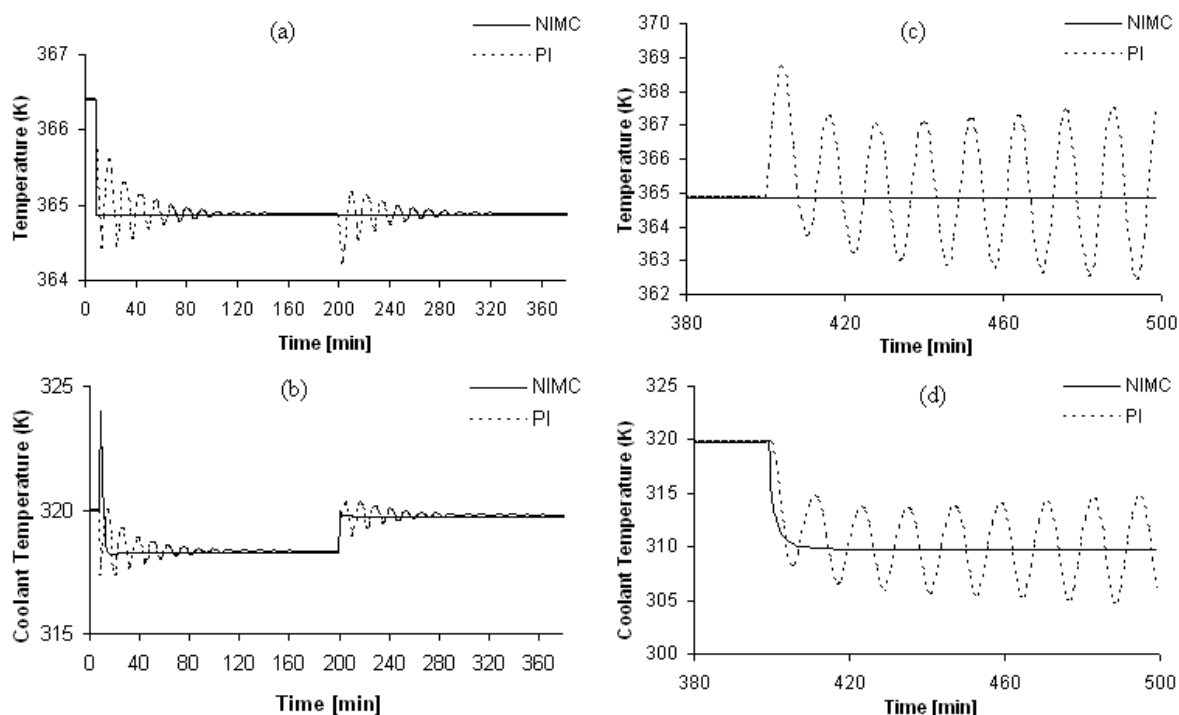


FIG. 13 PROCESS AND CONTROLLER OUTPUT PLOTS OF NIMC AND PI

The NIMC strategy supported by the state estimator is applied with the objectives of controlling the homopolymerization reactor under different conditions and the results are presented in terms of three cases. In the first case, the process is initially operated under stable operation. Then changes are introduced in temperature set point and the controller is applied to maintain the desired operation under different input disturbance conditions introduced at different timings. In the second case, the process is operated under oscillatory condition. The controller is applied to stabilize the process at the desired condition at a time during the open-loop oscillatory dynamics. In the third case, the process is operated under chaotic behaviour. The controller is applied to suppress the chaotic dynamics and to maintain the desired operation. The results of the NIMC strategy are also compared with those of a conventional PI controller. The tuning parameter in NIMC strategy is chosen as $\pi = 16.5$. The PI controller parameters are evaluated by using Ziegler and Nichols method and further tuned and set as $K_c = 1.76$ and $\pi = 4.0$. A sampling time of 1 sec is used for implementing the estimator and controller. For the first case, the process is initially at the stable steady state with $T = 366.4$ K and $T_c = 320$ K. At time $t = 8.3$ min, the temperature set-point is changed from 366.4 to 364.87 K and at $t = 200$ min, T_f is changed from 315.00 to 313.00 K while keeping the set-point as 364.87 K. The input and output profiles

corresponding these conditions are shown in Figs. 13(a) and 13(b), respectively. In the same case, at $t = 400$ min, the monomer volume fraction, v_{mf} is changed from 0.3 to 0.33 while keeping the set-point at 364.87 K and T_f at 313 K. The input and output profiles corresponding these conditions are shown in Figs. 13(c) and 13(d), respectively. Though the changes are introduced at different timings in one time scale, the results are represented in separate figures with two time scales for the sake of clarity. From these results, it is observed that the NIMC tracks the desired condition very quickly, whereas the PI controller exhibits oscillatory behaviour for a longer duration. The PI controller could even fail for change in v_{mf} as shown in Fig. 13(c). The NIMC effectively rejects the disturbance conditions and leads the process back to its desired operation in a very conservative fashion.

In the second case, the process is disturbed from its initial steady state by changing the T_c from 320 K to 318 K at $t = 8.3$ min. This condition makes the process to exhibit oscillatory behaviour. This open-loop behaviour of the system is shown in Fig. 14(a). During the oscillatory operation at $t = 217.4$ min, the controllers are applied to stabilize the operation and to maintain the desired response condition, which is set as 364.87 K for this case. The results of process output and controller output for both the controllers are shown in Figs. 14(b) and 14(c), respectively. From

these results, it is observed that both the controllers are able to track the process to the desired condition, but the NIMC has shown better performance by quickly suppressing the oscillations. In the third case, the process is exhibiting chaotic behaviour for $T=347.6$ K and $T_c = 318$ K.

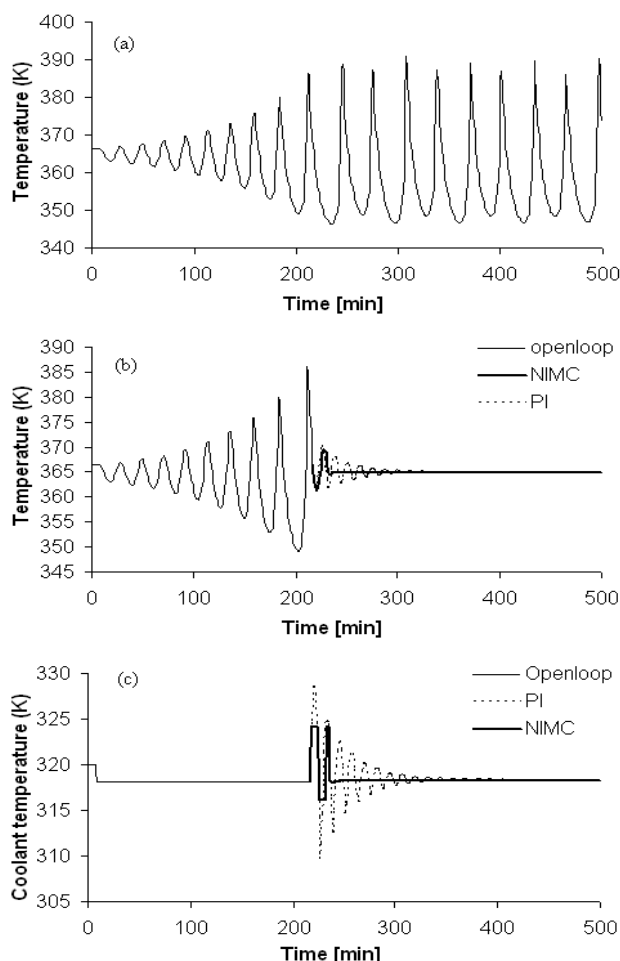


FIG. 14 OPEN LOOP AND CLOSED LOOP RESULTS: (A) OPEN-LOOP BEHAVIOUR (B) CONTROLLED OUTPUT (C) CONTROL INPUT

During the chaotic operation at $t = 240$ min, the controllers are applied to stabilize the operation and to maintain the desired response which is set as 364.87K for this case. The results of process output and controller output for both the controllers are shown in Figs. 15(a) and 15(b), respectively. Again, the NIMC has performed better by quickly suppressing the chaotic dynamics with less stringent control actions.

The results evaluated for both the chemical and polymerization reactors show the superior performance of the estimator based NIMC strategy over the conventional controllers. The performances of the controllers for different conditions are also expressed in terms of IAE values. The IAE values

shown in Table 3 correspond to the conditions for which the results are depicted in figures referred in Table. 3. These quantification results further confirm that the NIMC strategy is better suited for the control of nonlinear dynamical processes.

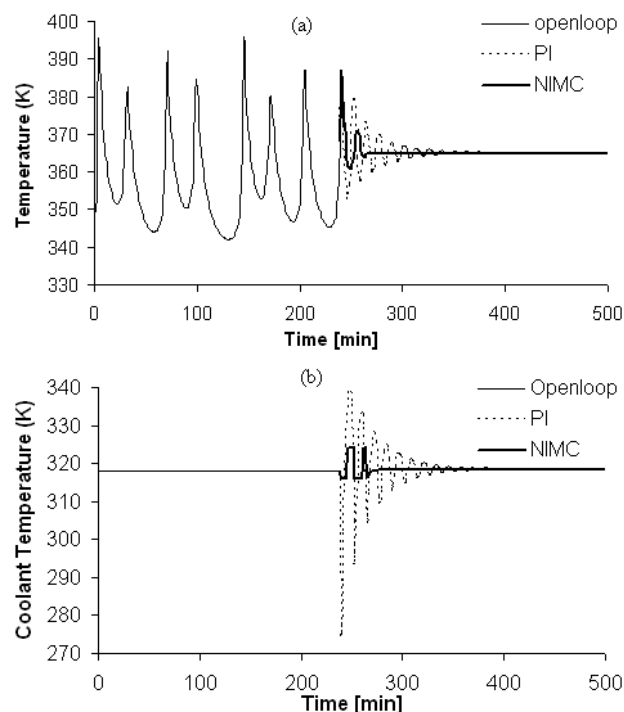


FIG. 15 OPEN LOOP AND CLOSED LOOP RESULTS: (A) CONTROLLED OUTPUT (B) CONTROL INPUT

TABLE 3 CONTROLLER'S PERFORMANCE

Chemical Reactor		
IAE		REFERENCE
NIMC	PID	
0.938	365.163	Fig. 3
0.748	72.763	Fig. 4
0.347	93.524	Fig. 5
7.121	83.042	Fig. 6
0.924	93.709	Fig. 7
6.852	118.350	Fig. 8
Polymer Reactor		
0.000985	174.193	Fig. 13
40.605	110.697	Fig. 14
138.626	339.425	Fig. 15

Conclusions

Complex dynamical systems can present the phenomena such as multiple steady state behaviour,

nonlinear oscillations and chaos. This phenomenon is usually analysed by means of dynamic mathematical models. The availability of such models can form a basis for the development of advanced nonlinear controllers for such systems. The nonlinear model based controllers require the process state information in the controller formulation. This necessitates the need for an estimator to provide the unmeasured process states desired by the controller. Thus, this work is focused towards the development of a nonlinear model based controller for complex dynamic systems, which is supported by a nonlinear model based estimator. A nonlinear internal model control (NIMC) strategy that incorporates the nonlinear model structure and the estimator dynamics in the control law is presented for the control of complex dynamical systems. The estimator is designed to provide the unmeasured process states that capture the fast changing nonlinear dynamics of the process to incorporate in the controller. The performance of the estimator supported NIMC strategy is evaluated by applying it for the control of a non-isothermal nonlinear chemical reactor and a homopolymerization reactor, which exhibit rich dynamical behaviour ranging from stable situations to chaos. The results evaluated under different conditions show the superior performance of the estimator based NIMC strategy over the conventional controllers.

Appendix A: Process Representation

The time varying model of the nonlinear process is represented by

$$\dot{x}(t) = f(x(t), t) + w(t), \quad x(0) = x_0 \quad (\text{A.1})$$

where $x(t)$ is n dimensional state vector, f is a nonlinear function of state $x(t)$ and $w(t)$ is an additive Gaussian noise with zero mean. The nonlinear measurement model with observation noise can be expressed as

$$y(t_k) = h(x(t_k)) + v(t_k) \quad (\text{A.2})$$

where h is a nonlinear function of state $x(t_k)$. The expected values of noise covariance matrices for the initial state $x(0)$, process noise $w(t)$ and observation noise $v(t_k)$ are given by the following relations,

$$\begin{aligned} P_0 &= E[(x_0 - x(0))(x_0 - x(0))^T] \\ Q(t) &= E[w(t) w^T(t)] \\ R(t_k) &= E[v(t_k) v^T(t_k)] \end{aligned} \quad (\text{A.3})$$

where P_0 is initial state covariance matrix, $Q(t)$ is process noise covariance matrix and $R(t_k)$ is observation noise covariance matrix. The EKF estimation algorithm is given in Appendix B.

Appendix B: State Estimation Algorithm

The extended Kalman filter is computed in two steps. The first is a prediction step, which is used to extrapolate the previous best estimates, and the second is a correction step by which the updated estimates are formed. Since prediction is based on process model, continuous prediction and discrete correction are employed in the estimation scheme.

Prediction equations: By starting with an initial estimate x_0 and its covariance P_0 at time zero and no measurements are taken between t_{k-1} and t_k , the propagating expression for the state estimate and its covariance from t_{k-1} to t_k are,

$$\dot{\hat{x}}(t/t_{k-1}) = f(\hat{x}(t/t_{k-1}), t) \quad (\text{B.1})$$

$$\begin{aligned} \dot{P}(t/t_{k-1}) &= F(\hat{x}(t/t_{k-1}), t)P(t/t_{k-1}) \\ &+ P(t/t_{k-1})F^T(\hat{x}(t/t_{k-1}), t) + Q(t) \end{aligned} \quad (\text{B.2})$$

where $F(\hat{x}(t/t_{k-1}), t)$ is the state transition matrix whose ij th element is given by

$$F(\hat{x}(t/t_{k-1}), t) = \frac{\partial f_i(x(t), t)}{\partial x_j(t)} \Big|_{x(t)=\hat{x}(t/t_{k-1})} \quad (\text{B.3})$$

The solution of the propagated estimate $\hat{x}(t/t_{k-1})$ and its covariance $P(t/t_{k-1})$ at time t_k are denoted by $\hat{x}(t_k/t_{k-1})$ and $P(t_k/t_{k-1})$. By using measurements at time t_k , the update estimate $\hat{x}(t_k/t_k)$ and its covariance $P(t_k/t_k)$ are computed.

Correction equations: The equations to obtain corrected estimates are:

$$\hat{x}(t_k/t_k) = \hat{x}(t_k/t_{k-1}) + K(t_k)[y(t_k) - h(\hat{x}(t_k/t_{k-1}))] \quad (\text{B.4})$$

$$P(t_k/t_k) = (I - K(t_k)H(x(t_k)))P(t_k/t_{k-1}) \quad (\text{B.5})$$

$$K(t_k) = \frac{P(t_k/t_{k-1})H^T(x(t_k))}{(H(x(t_k))P(t_k/t_{k-1})H^T(x(t_k)) + R)} \quad (\text{B.6})$$

where, $H(x(t_k)) = \frac{\partial h_i(x(t_k))}{\partial x(t_k)} \Big|_{x(t_k)=\hat{x}(t_k/t_{k-1})}$

The recursive initial conditions for state and covariance are:

$$\begin{aligned}\hat{x}(t_k/t_{k-1}) &= \hat{x}(t_k/t_k) \\ P(t_k/t_{k-1}) &= P(t_k/t_k)\end{aligned}\quad (\text{B.7})$$

Appendix C: Elements of F and H Matrices Chemical reactor

The nonlinear dynamic model of the reactor system in its dimensionless form is used in conjunction with the temperature measurements to estimate the reactor species concentrations. The design of soft sensor involves the following components:

State vector

The chemical species concentrations and the temperature define the state vector as

$$x = [x_1 \ x_2 \ x_3]^T \quad (\text{C.1})$$

State transition matrix

The elements f_{ij} of the state transition matrix, F are computed by taking the partial derivatives of $f(x)$ defined by (24) - (26) with respect to the state vector:

$$F = \begin{bmatrix} f_{11} & f_{12} & f_{13} \\ f_{21} & f_{22} & f_{23} \\ f_{31} & f_{32} & f_{33} \end{bmatrix} \quad (\text{C.2})$$

Measurement matrix

The measurement relation for temperature is

$$H = [0 \ 0 \ 1] \quad (\text{C.3})$$

The temperature state equation, (26) in its discrete form is used as the nonlinear measurement equation, $h(x)$. The elements of the measurement transition matrix, H_x are computed by taking the partial derivatives of $h(x)$ with respect to the state vector

$$H_x = [h_{11} \ h_{12} \ h_{13}] \quad (\text{C.4})$$

All these components are evaluated for chaotic reactor and used with the EKF estimator to obtain measured and unmeasured states of the reactor. The soft sensor uses the temperature data of every sampling time as measurements and provides the estimates of temperature as well as reactor species concentrations.

Polymer reactor

The nonlinear dynamic model of the VA homopolymerization system is used in conjunction with the temperature measurements to estimate the volume fraction of monomer, solvent, concentration of

initiator and reactor temperature. The design of soft sensor involves the following components:

State vector

The volume fraction of monomer, solvent, concentration of initiator and reactor temperature define the state vector as

$$x = [v_m \ v_s \ c_i \ T]^T \quad (\text{C.5})$$

State transition matrix

The elements f_{ij} of the state transition matrix, F are computed by taking the partial derivatives of $f(x)$ defined by (28) - (30) with respect to the state vector:

$$F = \begin{bmatrix} f_{11} & f_{12} & f_{13} & f_{14} \\ f_{21} & f_{22} & f_{23} & f_{24} \\ f_{31} & f_{32} & f_{33} & f_{34} \\ f_{41} & f_{42} & f_{43} & f_{44} \end{bmatrix} \quad (\text{C.6})$$

Measurement matrix

The measurement relation for temperature is

$$H = [0 \ 0 \ 0 \ 1] \quad (\text{C.7})$$

The temperature state equation, (30) in its discrete form is used as the nonlinear measurement equation, $h(x)$. The elements of the measurement transition matrix, H_x are computed by taking the partial derivatives of $h(x)$ with respect to the state vector

$$H_x = [h_{11} \ h_{12} \ h_{13} \ h_{14}] \quad (\text{C.8})$$

All these components are evaluated for homopolymerization reactor and used with the EKF estimator to obtain measured and unmeasured states of the reactor. The state estimator uses the temperature data of every sampling time as measurements and provides the estimates of temperature as well as reactor species concentrations.

Notation

B	heat of reaction parameter
c_i	initiator concentration in reactor, $gmol/l$
c_{if}	initiator feed concentration, $gmol/l$
c_p	heat capacity of reaction mixture, $cal/g \ ^\circ C$
c_{pf}	heat capacity of feed stream, $cal/g \ ^\circ C$
d_1, d_2, d_3	load disturbance in x_1, x_2, x_3
Da	Damkohler number
e	set point error

f	initiator dissociation efficiency
$-\Delta H_R$	heat of polymerization, $cal/gmol$
k	ratio of the activation energies for the series reaction
k_d	rate constant for initiator decomposition, l/s
k_p	rate constant for propagation, $l/gmol\ s$
k_t	rate constant for termination, $l/gmol\ s$
K_c	controller gain
$(MW)_m$	molecular weight of monomer, $g/gmol$
P	live radical concentration, $gmol/l$
$q_o q_i$	ratio of outlet to inlet volumetric flow rate
R_m	rate of consumption of monomer, $gmol/l\ min$
S	ratio of the rate constants for the series reaction
t	time, min
T	reactor temperature, K
T_c	coolant temperature, K
T_f	feed temperature, K
UA	overall heat transfer coefficient, $cal/min\ K$
u_t	manipulated variable
V	volume of the reactor, l
x_t	mole fraction of polymer
x_1	dimensionless concentration of species A
x_2	dimensionless concentration of species B
x_3	dimensionless temperature
x_{3c}	dimensionless coolant temperature
$x_1^{set}, x_2^{set}, x_3^{set}$	set point for variable x_1, x_2 and x_3
x_{1s}, x_{2s}, x_{3s}	steady state values of x_1, x_2 and x_3
y_i	weight fraction of respective components ($i=m, s, p$)

Greek symbols

α	ratio of heat effects for the series reaction
β	heat transfer coefficient
ε_0	initial controller gain
ε_1	initial controller gain
ε_A	activation number
θ	residence time, min

τ	dimensionless time (t/θ)
τ_D	time constant for derivative action
τ_I	time constant for integral action
v_m	volume fraction of monomer in reactor
v_{mf}	volume fraction of monomer in feed
ρ	density of reaction mixture, g/l
ρ_f	density of feed, g/l
$\rho_{f(T)}$	density of feed adjusted to reactor temperature, g/l
ρ_m	density of monomer at reactor conditions, g/l
ρ_{mf}	density of monomer at feed conditions, g/l
Subscripts	
m	monomer
s	solvent
p	polymer
f	feed

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